THE SPECTRUM OF THE FORCE-BASED QUASICONTINUUM OPERATOR FOR A HOMOGENEOUS PERIODIC CHAIN

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Abstract. We show under general conditions that the linearized force-based quasicontinuum (QCF) operator has a positive spectrum, which is identical to the spectrum of the quasinonlocal quasicontinuum (QNL) operator in the case of second-neighbour interactions. Moreover, we establish a bound on the condition number of a matrix of eigenvectors that is uniform in the number of atoms and the size of the atomistic region. These results establish the validity of and improve upon recent conjectures ([7, Conjecture 2] and [6, Conjecture 8]) which were based on numerical experiments.

As immediate consequences of our results we obtain rigorous estimates for convergence rates of (preconditioned) GMRES algorithms, as well as a new stability estimate for the QCF method.

1. Introduction

Quasicontinuum methods are a prototypical class of multiscale models that directly couple multiple modeling regions to reduce the computational complexity of modelling large atomistic systems. These methods are useful for computing the interaction of localized material defects such as crack tips or dislocations with long-range elastic fields of a crystalline material. The force-based quasicontinuum (QCF) method [3, 4, 21] partitions the material into two disjoint regions, the atomistic region and the continuum region. It assigns forces to the degrees of freedom within each region using only the respective model, be it atomistic or continuum. This simplifies the formulation of the method as no special interaction rules are needed near the atomistic-continuum interface. The simplicity of mixing forces combined with the lack of spurious interface forces (so-called "ghost forces") make the force-based method a popular approach, and this technique is widely applied in the multiscale literature [1, 2, 3, 11, 13, 21, 22].

A potential drawback of the QCF method is that it does not derive from an energy (as it generally produces a non-conservative field). While the practical implications of this fact are still under investigation, it is already clear that the analysis of the QCF method poses formidable challenges. A series of recent articles has been devoted to its study [6, 7, 8]. For example, it was shown in [7, 8] that the linearized QCF operator is not positive definite, and that it is not uniformly stable (in the number of atoms and the size of the atomistic region) in discrete variants of most Sobolev spaces.

Date: April 21, 2010.

2000 *Mathematics Subject Classification.* 65N12, 65N15, 70C20.

Key words and phrases. force-base atomistic/continuum coupling, stability, spectrum.

This work was supported in part by the EPSRC Critical Mass Programme "New Frontiers in the Mathematics of Solids" and the NSF Mathematical Sciences Postdoctoral Research Fellowship. This project was initiated by the authors at the OxMOS Workshop on Atomistic Models of Solids.

However, numerical experiments in [6, 7] showed some unexpected spectral properties. Conjecture 2 in [7] states that the spectrum of ℓ^2-eigenvalues of the linearized QCF operator is identical to that of the operator associated with the quasinonlocal QC method [23]. This is particularly surprising since the quasinonlocal QC method is energy-based, and thus indicates that the QCF operator is diagonalizable and that its spectrum is real. Conjecture 8 in [6] states that the condition number of a matrix of eigenvectors of the QCF operator grows at most logarithmically. This is an important fact for understanding the solution of the QCF equilibrium equations by the GMRES method.

The purpose of the present paper is to provide rigorous proofs for these numerical observations. We define the QCF method and introduce the necessary notation in Section 2. In Section 3 we establish all results for the case of next-nearest neighbour interactions as in the numerical experiments in [6, 7]. Then, in Section 4 we extend the results to the more technical case of finite-range interactions. In the case of finite-range interactions we cannot make the comparison between the spectra of the QCF and QNL operators. Instead, we prove that the spectrum of the QCF operator lies between the spectrum of the atomistic operator and the spectrum of the continuum operator (Theorem 12). We note, moreover, that we were able to construct a matrix of eigenvectors for the QCF operator whose condition number is bounded uniformly in the number of atoms and the size of the atomistic region. This result is in fact stronger than the conjectures made in [6]. Finally, in Section 5, we analyze variants of preconditioned QCF operators to obtain rigorous convergence rates for preconditioned GMRES methods as well as a new stability estimate.

2. Formulation of the QCF Method

For the sake of brevity, we will keep the introduction to the atomistic model and the various flavours of quasicontinuum approximations to an absolute minimum. We refer to [4, 6, 7, 8, 9, 14, 15, 16] for detailed discussions. Note, in particular, that we have left out the usual rescaling factor ε. This reduces the complexity of the notation and is justified since in this paper we are primarily concerned with algebraic aspects of quasicontinuum operators.

2.1. Notation for difference operators.

In this section, we summarize the notation and certain elementary results for some standard finite difference operators with periodic boundary conditions.

2.1.1. *Periodic domains.* We identify $\mathbb{R}^N$ with periodic infinite sequences as follows:

$$\mathbb{R}^N = \big\{ u \in \mathbb{R}^{\mathbb{Z}} : u_{\ell+N} = u_\ell \text{ for all } \ell \in \mathbb{Z} \big\}.$$

The ℓ^2-inner product on $\mathbb{R}^N$, and its associated norm, are defined as

$$\langle u, v \rangle = u^T v = \sum_{\ell=1}^{N} u_\ell v_\ell, \quad \text{and} \quad \|u\| = \sqrt{\langle u, u \rangle}.$$

We will frequently use a subspace $\mathcal{U} \subset \mathbb{R}^N$ of mean zero functions,

$$\mathcal{U} = \big\{ u \in \mathbb{R}^N : \langle u, e \rangle = 0 \big\},$$

where $e = (1)_{\ell\in\mathbb{Z}} \in \mathbb{R}^N$.

The orthogonal projection onto $\mathcal{U}$ is denoted $P_{\mathcal{U}} : \mathbb{R}^N \to \mathbb{R}^N$,

$$(P_{\mathcal{U}}u)_\ell = u_\ell - \frac{1}{N}\sum_{k=1}^{N} u_k,$$

or, in matrix notation,

$$P_{\mathcal{U}} = I - \tfrac{1}{N} e \otimes e. \tag{1}$$

2.1.2. *The backward difference operator.* The difference operator $D : \mathbb{R}^N \to \mathbb{R}^N$ is defined by

$$Du_\ell = (Du)_\ell = u_\ell - u_{\ell-1}.$$

We note that $\mathrm{rg}(D) = \mathcal{U}$ and $\ker(D) = \mathrm{span}\{e\}$ where rg denotes the range and ker denotes the kernel of an operator. We also remark that, here and throughout, unless specifically stated otherwise, we will not distinguish between an operator and its associated matrix representation in $\mathbb{R}^{N\times N}$.

2.1.3. *The discrete Laplace operator.* The second generic operator that we will encounter is the negative Laplace operator $L : \mathbb{R}^N \to \mathbb{R}^N$,

$$Lu_\ell = (Lu)_\ell = -u_{\ell-1} + 2u_\ell - u_{\ell+1}.$$

As for the difference operator, $\mathrm{rg}(L) = \mathcal{U}$ and $\ker(L) = \mathrm{span}\{e\}$.

Using summation by parts, we obtain

$$\langle Lu, v\rangle = \langle Du, Dv\rangle,$$

which implies that $L = D^T D$ and hence $L = L^T$. Since $Le = 0$, we have the identities

$$LP_{\mathcal{U}} = P_{\mathcal{U}}L = L. \tag{2}$$

We also note that $\|L\| \le 4$, and that this bound is attained for even N, as well as in the limit $N \to \infty$.

Since L is singular, we also define the modified negative Laplace operator

$$L_1 = L + e \otimes e = L + (I - P_{\mathcal{U}}), \tag{3}$$

so that $L_1 u = Lu$ if $u \in \mathcal{U}$ and $L_1 e = e$. This operator is invertible and satisfies

$$L_1^{-1}L = LL_1^{-1} = P_{\mathcal{U}}.$$

2.1.4. *The translation operator.* The translation operator $T : \mathbb{R}^N \to \mathbb{R}^N$ is defined by

$$Tu_\ell = (Tu)_\ell = u_{\ell+1}. \tag{4}$$

T is an orthogonal operator, i.e., $T^T T = I$ and its eigenbasis can be written explicitly as

$$Tw_k = \lambda_k w_k, \quad \lambda_k = e^{\frac{i2\pi k}{N}}, \quad (w_k)_\ell = e^{\frac{i2\pi k\ell}{N}} \quad \text{for } 1 \le k \le N. \tag{5}$$

The eigenvalues of T are located on the unit circle $\mathcal{T} := \{t \in \mathbb{C} : \ |t| = 1\}$ and, in the limit $N \to \infty$, are dense in $\mathcal{T}$.

We remark that we can write the difference operator D and the negative Laplace operator as Laurent polynomials in T: $D = p_D(T)$ and $L = p_L(t)$ where

$$p_D(t) = (1 - t^{-1}), \quad \text{and} \quad p_L(t) = (-t + 2 - t^{-1}).$$

In general, if $p(t)$ is a polynomial, then the spectrum of the operator $p(T)$ is $\{p(\lambda_k) : 1 \le k \le N\}$, and the eigenvectors are the same as for T. Since T is a normal operator, all polynomials $p(T)$ are also normal.

Finally, we note that $Te = e$, which implies that T or any polynomial of T commutes with $e \otimes e$. In particular, this implies that all polynomials in T (e.g., L, D) and the operators L_1 and $P_{\mathcal{U}}$ commute.

2.2. **The linearized atomistic operators.** We consider an atomistic model problem with periodic boundary conditions. We let $\mathcal{U}$ be the set of admissible displacements of an N-periodic chain: the set of all N-periodic displacements with mean zero. The latter condition is necessary to ensure that the systems of equations that we consider are well posed. If $F > 0$ is a fixed *macroscopic strain*, then the energy (per period) of the atomistic chain subject to a displacement $u \in \mathbb{R}^N$ is given by

$$\mathcal{E}^{\mathrm{a}}(u) = \sum_{r=1}^{R} \sum_{\ell=1}^{N} \phi\big(rF + (u_\ell - u_{\ell-r})\big)$$

where $\phi \in \mathrm{C}^2(0, +\infty)$ is a pair interaction potential, for example, a Lennard–Jones or Morse potential, and $R \in \mathbb{N}$, $R \ge 2$, can be thought of as a discrete cutoff radius. (Note that, even though we have defined $\mathcal{E}^{\mathrm{a}}$ for all $u \in \mathbb{R}^N$, only $u \in \mathcal{U}$ are admitted in the solution of the minimization problem.)

The Cauchy–Born or local quasicontinuum (QCL) approximation of $\mathcal{E}^{\mathrm{a}}$ is the functional

$$\mathcal{E}^{\mathrm{c}}(u) = \sum_{\ell=1}^{N} W\big(F + (u_\ell - u_{\ell-1})\big) = \sum_{\ell=1}^{N} W\big(F + Du_\ell\big),$$

where W is the *Cauchy–Born stored energy function*, $W(s) = \sum_{r=1}^{R} \phi(rs)$.

Our analysis in the present paper concerns properties of the Hessians $L^{\mathrm{a}} = D^2\mathcal{E}^{\mathrm{a}}(0)$ and $L^{\mathrm{c}} = D^2\mathcal{E}^{\mathrm{c}}(0)$ and the quasicontinuum operators that we derive from them. For future reference we write out L^{a} and L^{c} explicitly,

$$(L^{\mathrm{a}}u)_\ell = \sum_{r=1}^{R} \phi''_{rF}(-u_{\ell+r} + 2u_\ell - u_{\ell-r}), \qquad \text{and} \tag{6}$$

$$(L^{\mathrm{c}}u)_\ell = \sum_{r=1}^{R} \phi''_{rF} r^2(-u_{\ell+1} + 2u_\ell - u_{\ell-1}) = W''_F\,(Lu)_\ell, \tag{7}$$

where the constants ϕ''_{rF} and W''_F are given by

$$\phi''_{rF} = \phi''(rF) \quad \text{and} \quad W''_F = W''(F) = \sum_{r=1}^{R} \phi''_{rF} r^2.$$

We understand both L^{a} and L^{c} as linear operators from $\mathbb{R}^N$ to $\mathbb{R}^N$, defined by the above formulas, but are primarily interested in their properties on $\mathcal{U}$. For example, we note that if $\phi''_F > 0$ and $W''_F > 0$, then both are positive definite on $\mathcal{U}$ and in particular invertible (see [7, Eq. (2.2) and Sec. 2.2] and [5, Prop. 1 and Prop. 2] for the next-nearest neighbour case, and [10] for finite range), however, both operators have a non-trivial kernel that contains e. For the continuum operator, L^{c}, the stability condition $W''_F > 0$ is sharp, that

is, L^{c} is positive definite if and only if $W_F'' > 0$. We work to prove our spectral results on L^{qcf} up to this sharp stability criterion.

2.3. **The force-based quasicontinuum method.** The force-based quasicontinuum (QCF) method is obtained by mixing the forces from the atomistic and the continuum model. To this end, we define atomistic and continuum regions $\mathcal{A}$ and $\mathcal{C}$ that satisfy

$$\mathcal{A} \cup \mathcal{C} = \{1, \dots, N\} \qquad \text{and} \qquad \mathcal{A} \cap \mathcal{C} = \emptyset. \tag{8}$$

We define the QCF forces

$$F_\ell^{\mathrm{qcf}}(u) = \begin{cases} -\frac{\partial \mathcal{E}^{\mathrm{a}}(u)}{\partial u_\ell}, & \text{if } \ell \in \mathcal{A}, \\ -\frac{\partial \mathcal{E}^{\mathrm{c}}(u)}{\partial u_\ell}, & \text{if } \ell \in \mathcal{C}. \end{cases}$$

Linearization of the nonlinear QCF operator $F(u) = (F_\ell^{\mathrm{qcf}}(u))_{\ell=1}^N$ at $u = 0$, yields the *linear QCF operator* (or simply, *QCF operator*), $L^{\mathrm{qcf}} : \mathbb{R}^N \to \mathbb{R}^N$,

$$(L^{\mathrm{qcf}} u)_\ell = \begin{cases} (L^{\mathrm{a}} u)_\ell, & \text{if } \ell \in \mathcal{A}, \\ (L^{\mathrm{c}} u)_\ell, & \text{if } \ell \in \mathcal{C}, \end{cases} \tag{9}$$

which is the focus of our studies in the present paper.

Unfortunately, L^{qcf} as defined above, does not map $\mathcal{U}$ to $\mathcal{U}$, hence we will normally consider the projected QCF operator (see [7, Sec. 2.3] for more detail)

$$L_0^{\mathrm{qcf}} = P_{\mathcal{U}} L^{\mathrm{qcf}}.$$

To conclude this section we represent L^{qcf} in a more compact way. By considering the characteristic function of $\mathcal{A}$,

$$\chi_\ell = \begin{cases} 1, & \text{if } \ell \in \mathcal{A}, \\ 0, & \text{if } \ell \in \mathcal{C}, \end{cases}$$

and the associated diagonal operator $X : \mathbb{R}^N \to \mathbb{R}^N$,

$$(Xu)_\ell = \chi_\ell u_\ell,$$

we can write L^{qcf} in the form

$$L^{\mathrm{qcf}} = [1 - X] L^{\mathrm{c}} + X L^{\mathrm{a}} = L^{\mathrm{c}} + X[L^{\mathrm{a}} - L^{\mathrm{c}}]. \tag{10}$$

2.4. **The quasinonlocal quasicontinuum method.** The second atomistic/continuum hybrid scheme that will feature prominently in our investigations is the *quasinonlocal quasicontinuum (QNL) method* [23]. We note that the QNL method is only defined for second-neighbour interaction range (i.e., $R = 2$). Extensions to further neighbours exist [9, 12, 20], but we only use the version up to second neighbours in this paper. The QNL method is conservative with energy functional

$$\begin{aligned} \mathcal{E}^{\mathrm{qnl}}(u) = &\sum_{\ell \in \mathcal{A} \cup \mathcal{C}} \phi\big(F + (u_\ell - u_{\ell-1})\big) + \sum_{\ell \in \mathcal{A}} \phi\big(2F + (u_{\ell+1} - u_{\ell-1})\big) \\ &+ \sum_{\ell \in \mathcal{C}} \frac{1}{2} \Big\{ \phi\big(2F + 2(u_\ell - u_{\ell-1})\big) + \phi\big(2F + 2(u_{\ell+1} - u_\ell)\big) \Big\}. \end{aligned}$$

The linearized QNL operator is the Hessian of $\mathcal{E}^{\rm qnl}$ at $u = 0$, that is, $L^{\rm qnl} = D^2\mathcal{E}^{\rm qnl}(0)$. The operator $L^{\rm qnl} : \mathbb{R}^N \to \mathbb{R}^N$, is most easily written in variational form [5, Sec. 3.3],

$$\langle L^{\rm qnl} u, v\rangle = W''_F \sum_{\ell\in\mathcal{A}\cup\mathcal{C}} Du_\ell Dv_\ell - \phi''_{2F} \sum_{\ell\in\mathcal{A}} Lu_\ell Lv_\ell. \tag{11}$$

Based on this representation one can show that, if $W''_F > 0$ and $\phi''_F > 0$, then $L^{\rm qnl}$ is positive definite on $\mathcal{U}$ (see [5, Prop. 3] for the case when $\phi''_{2F} \le 0$; the case $\phi''_{2F} > 0$ is trivial).

3. The ℓ^2-Spectrum of the Second-Neighbour $L^{\rm qcf}$ Operator

In [7] the invertibility of the QCF operator was investigated analytically and numerically, and several interesting numerical observations were left as conjectures. Similar observations were also used in [6] to study the performance of iterative solution methods for the QCF operator. In the present section we rigorously establish some of the most fundamental of these conjectures in the next-nearest neighbour case. We will then extend the results, to finite range interactions in Section 4.

3.1. **Similarity of $L_0^{\rm qcf}$ and $L^{\rm qnl}$.** In [6, 7] it was observed in numerical experiments that the spectra of $L_0^{\rm qcf}$ and $L^{\rm qnl}$ coincide. In this section we provide a rigorous proof by explicitly constructing a similarity transformation between $L_0^{\rm qcf}$ and $L^{\rm qnl}$. The main ideas, after which the proof will be straightforward, are the following two new representations of the $L^{\rm qcf}$ and $L^{\rm qnl}$ operators.

Proposition 1. *Let $R = 2$, then $L^{\rm qcf}$ and $L^{\rm qnl}$ have, respectively, the representations*

$$L^{\rm qcf} = W''_F L - \phi''_{2F} X L^2, \qquad \textit{and} \tag{12}$$

$$L^{\rm qnl} = W''_F L - \phi''_{2F} L X L. \tag{13}$$

Proof. We begin by noting that, for $R = 2$, the operators $L^{\rm a}$ and $L^{\rm c}$ may be written as

$$L^{\rm a} = \phi''_F L + \phi''_{2F}[4L - L^2] = W''_F L - \phi''_{2F} L^2,$$
$$L^{\rm c} = \phi''_F L + \phi''_{2F}[4L] = W''_F L.$$

Using these formulas, the operator $L^{\rm qcf}$ (as defined in (9)) can be written in terms of the atomistic and the continuum operators (10) as

$$L^{\rm qcf} = XL^{\rm a} + [I - X]L^{\rm c} = X\left[W''_F L - \phi''_{2F} L^2\right] + [I - X]\left[W''_F L\right].$$

From this we immediately obtain (12).

To rewrite the QNL operator, we note that we can write (11) as

$$\begin{aligned}\langle L^{\rm qnl} u, v\rangle &= W''_F\langle Du, Dv\rangle - \phi''_{2F}\langle XLu, Lv\rangle \\ &= W''_F\langle D^T Du, v\rangle - \phi''_{2F}\langle LXLu, v\rangle,\end{aligned}$$

for all $u, v \in \mathbb{R}^N$, and we therefore obtain (13). ∎

Based on (12) and (13) we will deduce the similarity of the QCF and QNL operators. Since L is not invertible, we introduce the nonsingular operator $L_1 : \mathbb{R}^N \to \mathbb{R}^N$ defined by (3). The following result confirms Conjecture 2 in [7] (a related conjecture with different boundary conditions is Conjecture 6 in [6]).

Theorem 2 (Similarity of $L_0^{\rm qcf}$ and $L^{\rm qnl}$). *If $R = 2$ then the operators $L_0^{\rm qcf}$ and $L^{\rm qnl}$ are similar, with similarity transformation L_1 defined by (3):*

$$L_0^{\rm qcf} = L_1^{-1} L^{\rm qnl} L_1.$$

In particular, the spectra of $L_0^{\rm qcf}$ and $L^{\rm qnl}$ coincide.

Proof. Using formulas (2), (12), and (13), a straightforward computation yields the desired identity:

$$\begin{aligned} L_1 L_0^{\rm qcf} &= L_1 P_{\mathcal{U}} L^{\rm qcf} = L L^{\rm qcf} \\ &= W_F'' L L - \phi_{2F}'' L X L^2 \\ &= [W_F'' L - \phi_{2F}'' L X L] L_1 = L^{\rm qnl} L_1. \end{aligned}$$

□

3.2. **Condition number of the ℓ^2 eigenbasis.** Since $L^{\rm qnl}$ is self-adjoint, there exists an orthonormal matrix $V^{\rm qnl} \in \mathbb{R}^{N\times N}$, and a diagonal matrix Λ containing the eigenvalues of $L^{\rm qnl}$, such that

$$L^{\rm qnl} V^{\rm qnl} = V^{\rm qnl} \Lambda. \tag{14}$$

Note in particular that Λ also contains the zero eigenvalue. Since the operators $L^{\rm qnl}$ and $L_0^{\rm qcf}$ are similar, there exists also an invertible operator $V^{\rm qcf} \in \mathbb{R}^{N\times N}$ such that

$$L_0^{\rm qcf} V^{\rm qcf} = V^{\rm qcf} \Lambda.$$

As suggested by Theorem 2, a possible choice for the eigenvectors is $L_1^{-1} V^{\rm qnl}$, since in that case we have

$$L_0^{\rm qcf}\, L_1^{-1} V^{\rm qnl} = L_1^{-1} L^{\rm qnl} V^{\rm qnl} = L_1^{-1} V^{\rm qnl}\, \Lambda.$$

However, $\mathrm{cond}(L_1^{-1} V^{\rm qnl}) = \mathrm{cond}(L_1^{-1}) = O(N^2)$, which is much worse than the numerical observations in [7] and suggests a poor scaling of the eigenvectors.

To produce a better eigenbasis, it is important to note that the choice of eigenvectors is not unique even after fixing the ordering as we are always free to rescale them. This turns out to be a crucial ingredient in our following construction of an eigenbasis with a uniformly bounded condition number. The following result is inspired by Figure 4.2 in [7] and Conjecture 8 in [6]. It does not precisely confirm these, but establishes a closely related and in fact stronger result.

Theorem 3. *Suppose that $R = 2$, then the operator $V^{\rm qcf} : \mathbb{R}^N \to \mathbb{R}^N$,*

$$V^{\rm qcf} = [W_F'' I - \phi_{2F}'' P_{\mathcal{U}} X L] V^{\rm qnl}, \tag{15}$$

diagonalizes $L_0^{\rm qcf}$, that is, $L_0^{\rm qcf} V^{\rm qcf} = V^{\rm qcf} \Lambda$, where Λ is the diagonal matrix of eigenvalues associated with $L^{\rm qnl}$ (14). Moreover, if $W_F'' > 0$ and $\phi_F'' > 0$ then $\mathrm{cond}(V^{\rm qcf})$ is bounded above by a constant that depends on ϕ_{2F}''/W_F'', but is independent of N and $\mathcal{A}$.

Remark 1. The choice of V^{qcf} is motivated by the following calculation. Starting with the similarity result of Theorem 2, we derive

$$L_0^{\mathrm{qcf}} = L_1^{-1} L^{\mathrm{qnl}} L_1 = L_1^{-1} V^{\mathrm{qnl}} \Lambda (V^{\mathrm{qnl}})^T L_1,$$

and we scale the eigenvectors by Λ, which gives

$$\begin{aligned} L_1^{-1} V^{\mathrm{qnl}} \Lambda &= L_1^{-1} V^{\mathrm{qnl}} \Lambda [V^{\mathrm{qnl}}]^T V^{\mathrm{qnl}} = L_1^{-1} L^{\mathrm{qnl}} V^{\mathrm{qnl}} \\ &= L_1^{-1} [W_F'' L - \phi_{2F}'' L X L] V^{\mathrm{qnl}} = [W_F'' P_{\mathcal{U}} - \phi_{2F}'' P_{\mathcal{U}} X L] V^{\mathrm{qnl}}. \end{aligned}$$

This is equivalent to the choice of V^{qcf} in (15) when restricted to $\mathcal{U}$. □

Proof of Theorem 3. Step 1: Diagonalization. In a straightforward computation we obtain

$$\begin{aligned} L_0^{\mathrm{qcf}} V^{\mathrm{qcf}} &= \big[W_F'' L - \phi_{2F}'' P_{\mathcal{U}} X L^2\big] \big[W_F'' I - \phi_{2F}'' P_{\mathcal{U}} X L\big] V^{\mathrm{qnl}} \\ &= \big[W_F'' I - \phi_{2F}'' P_{\mathcal{U}} X L\big] \big[W_F'' L - \phi_{2F}'' L X L\big] V^{\mathrm{qnl}} \\ &= \big[W_F'' I - \phi_{2F}'' P_{\mathcal{U}} X L\big] V^{\mathrm{qnl}} \Lambda \\ &= V^{\mathrm{qcf}} \Lambda. \end{aligned}$$

Step 2: Estimating $\mathrm{cond}(V^{\mathrm{qcf}})$. We now assume that $W_F'' > 0$ and $\phi_F'' > 0$. To estimate $\mathrm{cond}(V^{\mathrm{qcf}})$ we can ignore the positive constant multiple W_F'' as well as the orthonormal matrix V^{qnl}, that is, we have

$$\begin{aligned} \mathrm{cond}(V^{\mathrm{qcf}}) = \mathrm{cond}(A) &= \|A\| \, \|A^{-1}\|, \\ \text{where} \qquad A &= I - \alpha P_{\mathcal{U}} X L, \end{aligned} \tag{16}$$

with constant $\alpha = \frac{\phi_{2F}''}{W_F''}$, and the convention $\|A^{-1}\| = +\infty$ if A is not invertible. We note that the condition $\phi_F'', W_F'' > 0$ implies that $\alpha < 1/4$.

Elementary estimates give the upper bound

$$\|A\| \le 1 + |\alpha| \|P_{\mathcal{U}}\| \|X\| \|L\| = 1 + 4|\alpha|. \tag{17}$$

We similarly get the lower bound

$$\|Au\| \ge 1 - |\alpha| \|P_{\mathcal{U}}\| \|X\| \|L\| = 1 - 4|\alpha| \qquad \text{for all } \|u\| = 1, \tag{18}$$

which gives an estimate for $\|A^{-1}\|$ whenever $W_F'' + 4\phi_{2F}'' > 0$. In the following we prove a bound for $\|A^{-1}\|$ that holds whenever $W_F'' > 0$, that is, up to the sharp stability limit, which is a more involved result.

To estimate $\|A^{-1}\|$ we use the facts that (i) $\|A^{-1}\| = \|A^{-T}\|$, and (ii) if

$$\|A^T u\| \ge \gamma_0 \|u\| \qquad \forall u \in \mathbb{R}^N,$$

for some constant $\gamma_0 > 0$, then A^T is invertible and $\|A^{-T}\| \le 1/\gamma_0$. In Lemma 4 we establish precisely this fact, assuming that $\alpha < 1/4$, with a constant γ_0 that depends only on α but not on N or $\mathcal{A}$. □

A generalization of the following technical lemma used in the previous proof will also be required in the finite range interaction case. It follows from Lemma 11 by choosing $Z = I$.

Lemma 4. *Let $\alpha < 1/4$, then there exists a constant $\gamma_0 > 0$, which depends on α but is independent of N and of $\mathcal{A}$, such that*

$$\big\|[I - \alpha P_{\mathcal{U}} X L]^T u\big\| \geq \gamma_0 \|u\| \qquad \forall u \in \mathbb{R}^N.$$

Remark 2. From the proof of Lemma 11 we see that, in the case $\phi''_{2F} \leq 0$, the constant γ_0 is explicitly given by

$$\gamma_0^2 = 1 + 8\alpha^2 - 4\sqrt{\alpha^2 + 4\alpha^4}, \tag{19}$$

where $\alpha = \phi''_F / W''_F$, and the resulting condition number estimate by

$$\mathrm{cond}(V^{\mathrm{qcf}}; \mathcal{U})^2 \leq \frac{(1 + 4|\alpha|)^2}{1 + 8\alpha^2 - 4\sqrt{\alpha^2 + 4\alpha^4}} =: c(\alpha)^2.$$

If ϕ''_{2F} is moderate but $W''_F \to 0$, then $\alpha \to -\infty$. A brief calculation shows that in this limit $c(\alpha)$ behaves asymptotically like

$$c(\alpha) \sim 2^{5/2}\alpha^2 + O(|\alpha|^{3/2}) \qquad \text{as} \quad \alpha \to \infty. \qquad \square$$

4. Finite Range Interactions

In this section we extend the results of Section 3 to the case of finite range interactions (i.e., with arbitrary finite R). We begin by stating a simplified formulation of our main results. We note, however, that our actual results are more general than the following theorem. In particular, we can replace the assumption $\phi''_{rF} \leq 0$, $r \geq 2$, by a more general condition. This theorem will be proved in Section 4.4.

Theorem 5. *Suppose that $\phi''_{rF} \leq 0$ for $2 \leq r \leq R$ and that $\phi''_{RF} \neq 0$.*

(i) There exists an operator $V^{\mathrm{qcf}} : \mathbb{R}^N \to \mathbb{R}^N$, which diagonalizes L_0^{qcf}, that is,

$$L_0^{\mathrm{qcf}} V^{\mathrm{qcf}} = V^{\mathrm{qcf}} \Lambda,$$

where Λ is a diagonal real matrix of eigenvalues $(\lambda_j)_{j=1}^N$.

(ii) If $W''_F > 0$ then V^{qcf} is invertible and $\mathrm{cond}(V^{\mathrm{qcf}})$ is bounded above by a constant that depends on the coefficients ϕ''_{rF}, $r = 1, \dots, R$, but is independent of N and $\mathcal{A}$.

(iii) If $W''_F > 0$ and if the eigenvalues are ordered, then

$$\lambda_j^{\mathrm{c}} \leq \lambda_j \leq \lambda_j^{\mathrm{a}},$$

where $(\lambda_j^{\mathrm{c}})_{j=1}^N$ and $(\lambda_j^{\mathrm{a}})_{j=1}^N$ denote the ordered eigenvalues of, respectively, L^{c} and L^{a}. In particular, we have the bounds

$$\lambda_1 = 0, \quad \text{and} \quad 4W''_F \sin^2\left(\tfrac{\pi}{N}\right) \leq \lambda_j \leq 4\phi''_F \quad \text{for } j = 2, \dots, N.$$

4.1. **Symmetrization of $L^{\rm qcf}$.** We recall from (10) the definition of the finite range QCF operators,

$$L^{\rm qcf} = L^{\rm c} + X[L^{\rm a} - L^{\rm c}], \quad \text{and} \quad L_0^{\rm qcf} = L^{\rm c} + P_{\mathcal{U}} X[L^{\rm a} - L^{\rm c}],$$

where $L^{\rm a}$ and $L^{\rm c}$ are, respectively, the atomistic and the continuum operators defined in (6) and (7). In terms of the translation operator defined in (4), we can express $L^{\rm a}$ and $L^{\rm c}$ as

$$L^{\rm c} = \sum_{r=1}^{R} r^2 \phi''_{rF}\big[-T + 2I - T^{-1}\big], \quad \text{and} \quad L^{\rm a} = \sum_{r=1}^{R} \phi''_{rF}\big[-T^r + 2I - T^{-r}\big]. \tag{20}$$

To show that $L_0^{\rm qcf}$ is diagonalizable, we aim to construct a matrix Y such that $Y L^{\rm qcf} Y^{-1}$ is symmetric. We first note that we can write the difference $L^{\rm a} - L^{\rm c}$ as a Laurent polynomial of the translation operator T:

$$\begin{aligned} L^{\rm a} - L^{\rm c} &= \sum_{r=2}^{R} \phi''_{rF}\big[(-T^r + 2I - T^{-r}) - r^2(-T + 2I - T^{-1})\big] \\ &= \sum_{r=2}^{R} \phi''_{rF}\big[(T^r - I)(T^{-r} - I) - r^2(T - I)(T^{-1} - I)\big]. \end{aligned}$$

Thus, if we define the Laurent polynomial

$$b(t) = \sum_{r=2}^{R} \phi''_{rF}\big[(t^r - 1)(t^{-r} - 1) - r^2(t-1)(t^{-1} - 1)\big] \quad \text{for } t \in \mathbb{C} \setminus \{0\}, \tag{21}$$

then we obtain $L^{\rm a} - L^{\rm c} = b(T)$. The crucial observation is the following: If we can factorize $b(t)$ as $b(t) = p(t)p(1/t)$ then we can choose $Y = p(T)$ to obtain

$$L^{\rm a} - L^{\rm c} = b(T) = p(T)p(T^{-1}) = p(T)p(T^T) = YY^T = Y^T Y, \tag{22}$$

and we immediately obtain

$$Y L^{\rm qcf} = Y L^{\rm c} + Y X\big[Y^T Y\big] = \big[L^{\rm c} + Y X Y^T\big] Y. \tag{23}$$

Here, we have used the fact that all operators that are polynomials in T commute. A similar result holds also for $L_0^{\rm qcf}$, though this would require further preparation. If Y were invertible (this will turn out to be false), then this would imply that $L^{\rm qcf}$ is similar to a symmetric, hence, normal matrix, and is therefore diagonalizable.

The desired polynomial factorization result is essentially the Riesz–Fèjer factorization lemma [18, Sec. 53], which we state and prove in a slightly more general form.

Lemma 6. *Let $b(t)$ be a Laurent polynomial with real coefficients such that $b(t) = b(1/t)$. Then there exists a polynomial $p(t)$ such that $b(t) = p(t)p(1/t)$.*

If, in addition, $b(t) \ge 0$ for all $t \in \mathcal{T} := \{t \in \mathbb{C} : |t| = 1\}$, then $p(t)$ can be chosen to have real coefficients.

Remark 3. In Lemma 6, if $b(t) \le 0$ on $\mathcal{T}$, then it can be factorized as $b(t) = -p(t)p(1/t)$, where $p(t)$ has real coefficients. □

Proof of Lemma 6. Let αt^{-R} be the leading term in $b(t)$ with $\alpha \neq 0$, then $a(t) := t^R b(t)$ is a polynomial with $a(0) \neq 0$. Moreover, a and b share the same roots, which we collect into a set Λ, so that

$$b(t) = \alpha t^{-R} \prod_{\lambda \in \Lambda} (t - \lambda)^{m(\lambda)},$$

where $m(\lambda)$ denotes the multiplicity of λ.

Next, we define the auxiliary polynomial

$$p_1(t) = \prod_{\lambda \in \Lambda, |\lambda| < 1} (t - \lambda)^{m(\lambda)}.$$

Since $b(t)$ has real coefficients it follows that $\lambda \in \Lambda$ if and only if $\bar{\lambda} \in \Lambda$, and $m(\lambda) = m(\bar{\lambda})$, and hence $p_1(t)$ also has real coefficients. We also note that

$$p_1(1/t) = \prod_{\lambda \in \Lambda, |\lambda| < 1} (-\lambda/t)^{m(\lambda)} \big(t - 1/\lambda\big)^{m(\lambda)}.$$

Since $b(t) = b(1/t)$, for each root λ with $|\lambda| > 1$, $1/\lambda$ is also a root, with the same multiplicity, and therefore we have

$$b(t) = p_1(t)\, p_1(1/t)\, b_1(t),$$

where

$$b_1(t) = \alpha_1 t^{-k_1} \prod_{\lambda \in \Lambda, |\lambda| = 1} (t - \lambda)^{m(\lambda)}$$

for some constants $\alpha_1 \in \mathbb{R}$ and $k_1 \in \mathbb{N}$. By construction, b_1 has real coefficients and $b_1(t) = b_1(1/t)$.

We will later assume that b has no roots on $\mathcal{T}$ except for $t = 1$, and for that case, the proof would be complete. To establish the lemma in its full generality, we now distinguish two cases.

Case 1: $b(t) \geq 0$ on $\mathcal{T}$. For $t \in \mathcal{T}$, we have $1/t = \bar{t}$, and hence, upon reordering the product in $p_1(1/t)$,

$$p_1(t)p_1(1/t) = \prod_{\lambda \in \Lambda, |\lambda| < 1} \Big[(t - \lambda)^{m(\lambda)} (\bar{t} - \bar{\lambda})^{m(\lambda)}\Big] > 0 \quad \text{for all } t \in \mathcal{T}.$$

Thus, if $b(t) \geq 0$ on $\mathcal{T}$, then we also have $b_1(t) \geq 0$ on $\mathcal{T}$. This implies that the multiplicity $m(\lambda)$ of all roots $\lambda \in \mathcal{T} \cap \Lambda$ is even. We can therefore define

$$p_2(t) = \prod_{\lambda \in \Lambda, |\lambda| = 1} (t - \lambda)^{m(\lambda)/2},$$

and argue similarly as above, to obtain that $p_2(t)$ has real coefficients and that

$$b_1(t) = \alpha_2 t^{-k_2} p_2(t) p_2(1/t) =: b_2(t) p_2(t) p_2(1/t),$$

for some constants $\alpha_2 \in \mathbb{R}$ and $k_2 \in \mathbb{N}$, and $b_2(t) = \alpha_2 t^{-k_2}$. We can again deduce that $b_2(t) = b_2(1/t)$ and that $b_2(t) \geq 0$ on $\mathcal{T}$, which implies that $k_2 = 0$ and $\alpha_2 \geq 0$. Thus, we obtain $p(t)$ by defining

$$p(t) = \sqrt{\alpha_2}\, p_1(t) p_2(t).$$

Case 2: $b(t) \not\geq 0$ on $\mathcal{T}$. In this case the multiplicity of roots $\lambda \in \mathcal{T}$ may be odd, and therefore we define

$$p_2(t) = \prod_{\lambda \in \Lambda, |\lambda|=1, \mathrm{Im}\lambda > 0} (t-\lambda)^{m(\lambda)}.$$

Thus, $p_2(t)$ contains all roots of $b_1(t)$ with positive imaginary part and $p_2(1/t)$ contains all roots of $b_1(t)$ with negative imaginary part. We are only left to find any roots at ± 1. Since $b_1(t) = b_1(1/t)$ it follows that these roots must be even (possibly $m(-1) = 0$), and hence we can define

$$p_3(t) = (t-1)^{m(1)/2}(t+1)^{m(-1)/2},$$

to obtain

$$b_1(t) = \alpha_2 t^{k_2} p_2(t) p_2(1/t) p_3(t) p_3(1/t)$$

for some constants $\alpha_2 \in \mathbb{R}$ and $k_2 \in \mathbb{Z}$. Arguing as before we find that $\alpha_2 > 0$ and $k_2 = 0$, and hence we obtain the result if we define

$$p(t) = \sqrt{\alpha_2}\, p_1(t) p_2(t) p_3(t). \qquad \square$$

For any Laurent polynomial $b(t)$ we call a polynomial $p(t)$ that satisfies $b(t) = p(t)p(1/t)$ a GRF-factorization (generalized Riesz–Fèjer factorization) of $b(t)$.

Since the Laurent polynomial $b(t)$ defined in (21) clearly satisfies the condition $b(t) = b(1/t)$, we have now indeed established (22) and (23). Thus, if Y were invertible, then we could deduce that L^{qcf} (and similarly L_0^{qcf}) is diagonalizable. Unfortunately, as follows from the next lemma, Y is always singular.

Lemma 7. *Let $p(t)$ be any GRF-factorization of the Laurent polynomial $b(t)$ defined in* (21)*, then there exists a polynomial $p_1(t)$ such that $p(t) = (t-1)^2 p_1(t)$. In particular, the operator $Y = p(T)$ can be rewritten as*

$$Y = LY_1 \qquad \textit{where} \quad Y_1 = -Tp_1(T).$$

Proof. It can be immediately seen from the definition of $b(t)$ that $b(1) = 0$ and, since $b(1) = p(1)^2$, it follows that $p(1) = 0$. Next, dividing $b(t)$ by $(t-1)(t^{-1}-1)$ we obtain

$$\begin{aligned}\frac{p(t)p(1/t)}{(t-1)(t^{-1}-1)} &= \frac{b(t)}{(t-1)(t^{-1}-1)} \\ &= \sum_{r=2}^{R} \phi''_{rF}\big[(1+t+\cdots+t^{r-1})(1+t^{-1}+\cdots+t^{-r+1}) - r^2\big],\end{aligned}$$

and hence

$$\frac{p(t)p(1/t)}{(t-1)(t^{-1}-1)}\bigg|_{t=1} = 0.$$

Thus, we see that 1 is also a (multiple) root of $\frac{p(t)p(1/t)}{(t-1)(t^{-1}-1)}$, and we can conclude that $p(t) = (t-1)^2 p_1(t)$ for some polynomial $p_1(t)$.

Upon rewriting the representation $p(t) = (t-1)^2 p_1(t)$ as

$$p(t) = \big[(t-1)(t^{-1}-1)\big]\big[-tp_1(t)\big] = \big[-t+2-t^{-1}\big]\big[-tp_1(t)\big]$$

we obtain $Y = p(t) = LY_1$. $\square$

Thus, as a consequence of Lemma 7, we see that Y is always singular. Nevertheless, in order to construct a similarity transformation to diagonalize $L_0^{\rm qcf}$, we can make a similar modification as in the next-nearest neighbour case, and simply replace L by its invertible variant L_1 defined in (3). Of course this still leaves us to verify that Y_1 is invertible, for which we will introduce conditions in Sections 4.2 and 4.4.

Proposition 8. *Let $p(t)$ be any GRF-factorization of $b(t)$, and let $Y = p(T) = LY_1$, as in Lemma 7, then*

$$[L_1Y_1]L_0^{\rm qcf} = \big[L^{\rm c} + YXY^T\big][L_1Y_1].$$

In particular, if Y_1 is invertible then $L_0^{\rm qcf}$ is diagonalizable.

Proof. We use (22) to represent $L^{\rm a} - L^{\rm c}$, the fact that polynomials of T and L_1 commute, and the fact that $P_{\mathcal{U}}L_1 = L_1P_{\mathcal{U}} = L$, to obtain

$$\begin{aligned}[L_1Y_1]L_0^{\rm qcf} &= [L_1Y_1]L^{\rm c} + Y_1[L_1P_{\mathcal{U}}]XLY_1Y_1^TL \\ &= L^{\rm c}[L_1Y_1] + Y_1LXLY_1^TP_{\mathcal{U}}[L_1Y_1] \\ &= \big[L^{\rm c} + Y_1LXLY_1^T\big]\,[L_1Y_1]. \end{aligned}$$ □

4.2. **Condition number of the ℓ^2 eigenbasis.** To investigate the invertibility of Y_1 we will study the Laurent polynomial

$$b_1(t) = \frac{b(t)}{\big[(t-1)(t^{-1}-1)\big]^2} \tag{24}$$

on the unit circle $\mathcal{T}$. It will quickly become apparent that $b_1(t)$ needs to be bounded away from zero on $\mathcal{T}$ in order to obtain invertibility of Y_1 and bounds on the inverse that are uniform in N and $\mathcal{A}$. Consequently, we focus on the case where $b(t)$ does not change sign on $\mathcal{T}$ (note that $b(t)$ is always real on $\mathcal{T}$). To show that this is a reasonable assumption we will, in Section 4.4, study the case of non-positive coefficients $\phi''_{rF} \le 0$ for $r = 2, \dots, R$, which is of particular interest in applications as this condition is satisfied for most practical interaction potentials. We will show that one can obtain bounds of the following type: *there exist positive constants β_0, β_1 such that*

$$\beta_0^2 \le |b_1(t)| \le \beta_1^2 \qquad \forall t \in \mathcal{T}. \tag{25}$$

Clearly, since $b(t)$ is real on $\mathcal{T}$, it is necessary that $b_1(t)$ does not change sign on $\mathcal{T}$, that is, either $b_1(t) > 0$ or $b_1(t) < 0$. If $b_1(t) > 0$ then the matrix Y_1 defined in Lemma 7 is real, however, if $b_1(t) < 0$ then it is imaginary. For the following analysis we prefer to construct a real coordinate transform.

According to Remark 3 and Lemma 7, we can choose a polynomial $p(t) = (t-1)^2p_1(t)$ with real coefficients such that

$$b(t) = \sigma p(t)p(1/t),$$

where $\sigma \in \{+1, -1\}$ is the sign of $b_1(t)$ on $\mathcal{T}$. Thus, if we (re-)define Y_1 accordingly as

$$Y_1 = -Tp_1(T) \tag{26}$$

then Proposition 8 implies that

$$[L_1 Y_1] L_0^{\rm qcf} = \big[L^{\rm c} + \sigma(LY_1)X(LY_1)^T\big][L_1 Y_1]. \tag{27}$$

Next, we show that (24) implies invertibility of Y_1, including explicit bounds. Beforehand, however, we make a brief remark on the connection of the sign of $b(t)$ and a relationship between $L^{\rm a}$ and $L^{\rm c}$.

Remark 4. The assumption $b_1(t) > 0$ on $\mathcal{T}$, or, more generally, $b(t) \geq 0$ on $\mathcal{T}$, implies that

$$\langle L^{\rm a} u, u\rangle \geq \langle L^{\rm c} u, u\rangle \qquad \forall u \in \mathbb{R}^N.$$

This follows simply from the fact that $L^{\rm a}$ and $L^{\rm c}$ share the same eigenvectors, and that the spectrum of $L^{\rm a} - L^{\rm c}$, which is contained in $b(\mathcal{T})$ is non-negative.

Conversely, if $b(t) \leq 0$ on $\mathcal{T}$ then, by the same argument,

$$\langle L^{\rm a} u, u\rangle \leq \langle L^{\rm c} u, u\rangle \qquad \forall u \in \mathbb{R}^N.$$

These observations are interesting in their own right, and will moreover lead to useful estimates on the eigenvalues of the QCF operator $L_0^{\rm qcf}$ in Section 4.3. □

Lemma 9. *Let Y_1 be defined as in* (26) *and suppose that $b(t)$ satisfies* (25)*, then Y_1 is invertible and we have the bounds*

$$\|Y_1\| \leq \beta_1, \quad \textit{and} \quad \|Y_1^{-1}\| \leq 1/\beta_0.$$

Proof. Let $p(t) = (t-1)^2 p_1(t)$ be a GRF-factorization of $\sigma b(t)$ with real coefficients, then $p_1(t)$ is a GRF-factorization of $b_1(t)$ with real coefficients. Hence, for $t \in \mathcal{T}$, we obtain

$$b(t) = p_1(t) p_1(\bar t) = |p_1(t)|^2,$$

which implies that

$$\beta_0 \leq |t p_1(t)| \leq \beta_1 \qquad \forall t \in \mathcal{T}. \tag{28}$$

By assumption, $Y_1 = -T p_1(T) =: q_1(T)$. Since T is unitary, this implies that Y_1 has an orthonormal eigenbasis and that the spectrum of Y_1 is contained in $q_1(\mathcal{T})$. This immediately gives

$$\|Y_1\| \leq \sup_{t \in \mathcal{T}} |t p_1(t)| \leq \beta_1.$$

Moreover, we have

$$\|Y_1^{-1}\|^{-1} = \inf_{\|u\|=1} \|Y_1 u\| \geq \inf_{t\in\mathcal{T}} |t p_1(t)| \geq \beta_0,$$

which gives the second bound. □

According to (27), and Lemma 9, we have

$$[L_1 Y_1] L_0^{\rm qcf} [L_1 Y_1]^{-1} = L^{\rm c} + \sigma [LY_1] X [LY_1]^T =: L^{\rm sym}, \tag{29}$$

that is, $L^{\rm qcf}$ and $L^{\rm sym}$ are similar matrices. Since $L^{\rm sym}$ is real and symmetric, there exists an orthogonal operator $V^{\rm sym} \in \mathbb{R}^{N\times N}$ such that

$$L^{\rm sym} = V^{\rm sym} \Lambda [V^{\rm sym}]^T,$$

where Λ is the diagonal matrix of eigenvalues of $L_0^{\rm qcf}$, and we obtain

$$L_0^{\rm qcf} = [Y_1^{-1} L_1^{-1} V^{\rm sym}] \Lambda [Y_1^{-1} L_1^{-1} V^{\rm sym}]^{-1},$$

that is, the operator $Y_1^{-1} L_1^{-1} V^{\rm sym}$ diagonalizes $L_0^{\rm qcf}$. As in the nearest neighbour case, the eigenbasis $Y_1^{-1} L_1^{-1} V^{\rm sym}$ is poorly scaled and would lead to an $O(N^2)$ condition number. However, the same argument as in Remark 1 shows how to rescale the basis to obtain the following theorem.

Theorem 10. *Suppose that the Laurent polynomial $b(t)$ defined in* (21) *satisfies* (25), *and let Y_1 be defined by* (26). *Then the operator $V^{\rm qcf} \in \mathbb{R}^{N \times N}$,*

$$V^{\rm qcf} = \big[W_F'' Y_1^{-1} + \sigma P_{\mathcal{U}} X Y_1^T L \big] V^{\rm sym}$$

diagonalizes $L_0^{\rm qcf}$, that is, $L_0^{\rm qcf} V^{\rm qcf} = V^{\rm qcf} \Lambda$, where Λ is a real diagonal matrix of eigenvalues.

Moreover, if $W_F'' > 0$, and if $\sigma \beta_1^2 / W_F'' > -1/4$, then $V^{\rm qcf}$ is invertible and $\mathrm{cond}(V^{\rm qcf})$ *is bounded above by a constant that depends only on W_F'', β_0, β_1, and, in particular is independent of N and $\mathcal{A}$.*

Proof. The proof of this result is very similar to the proof of Theorem 3, and hence we shall be fairly brief. First, we note that, by Lemma 9, the matrix Y_1 can be chosen to be invertible, and hence $V^{\rm qcf}$ is well-defined. Moreover, we recall that Y_1 is a polynomial in T and hence commutes with all operators that commute with T, such as other polynomials in T, the modified negative Laplace operator L_1, and the projection operator $P_{\mathcal{U}}$.

Step 1: Diagonalization. As in the computation in the proof of Theorem 3, we obtain

$$\begin{aligned}
L_0^{\rm qcf} V^{\rm qcf} &= \big[W_F'' L + \sigma P_{\mathcal{U}} X Y_1 Y_1^T L^2 \big] \big[W_F'' Y_1^{-1} + \sigma P_{\mathcal{U}} X Y_1^T L \big] V^{\rm sym} \\
&= \big[W_F'' Y_1^{-1} + \sigma P_{\mathcal{U}} X Y_1^T L \big] \big[W_F'' L + \sigma L Y_1 P_{\mathcal{U}} X Y_1^T L \big] V^{\rm sym} \\
&= \big[W_F'' Y_1^{-1} + \sigma P_{\mathcal{U}} X Y_1^T L \big] V^{\rm sym} \Lambda \\
&= V^{\rm qcf} \Lambda.
\end{aligned}$$

Step 2: Estimating $\mathrm{cond}(V^{\rm qcf})$. Suppose now that $W_F'' > 0$. As before, estimating $\|V^{\rm qcf}\|$ is straightforward. Using Lemma 9, we obtain

$$\|V^{\rm qcf}\| \le W_F'' \|Y_1^{-1}\| + \|P_{\mathcal{U}} X Y_1^T L\| \le W_F''/\beta_0 + 4\beta_1, \tag{30}$$

where β_0 and β_1 are the constants from (25).

To estimate $V^{\rm qcf}$ from below, we will use again the fact that $\|[V^{\rm qcf}]^{-1}\| = \|[V^{\rm qcf}]^{-T}\| \le 1/(W_F'' \tilde\gamma_0)$ where $\tilde\gamma_0 > 0$ satisfies

$$\|[V^{\rm qcf}]^T u\| \ge \tilde\gamma_0 \|u\| \qquad \forall u \in \mathbb{R}^N. \tag{31}$$

Writing out $(V^{\rm qcf})^T$ in full, we get

$$\begin{aligned}
[V^{\rm qcf}]^T &= W_F'' Y_1^{-T} [V^{\rm sym}]^T \big[I + \tfrac{\sigma}{W_F''} Y_1^T L Y_1 X P_{\mathcal{U}} \big] \\
&= W_F'' [V^{\rm sym}]^T Y_1^{-T} \big[I - \alpha Y_1^T L Y_1 X P_{\mathcal{U}} \big],
\end{aligned}$$

where $\alpha = -\sigma / W_F''$. If $\alpha \beta_1^2 < 1/4$, then we can use Lemma 11 below to deduce that

$$\big\| \big[I + \tfrac{\sigma}{W_F''} Y_1^T L Y_1 X P_{\mathcal{U}} \big] v \big\| \ge \gamma_0 \|v\| \qquad \forall v \in \mathbb{R}^N,$$

where γ_0 depends only on $\alpha\beta_1^2 = -\sigma\beta_1^2/W_F''$, but is independent of N and $\mathcal{A}$. This implies (31) with $\tilde\gamma_0 = W_F''\gamma_0/\beta_1$.

Combining (30) and (31) gives the stated result. □

Lemma 11. *Let $A = I - \alpha P_{\mathcal{U}} X Z^T L Z$, where $Z \in \mathbb{R}^{N\times N}$ commutes with $P_{\mathcal{U}}$, and where $\alpha \in \mathbb{R}$ satisfies*

$$-\infty < \alpha\|Z\|^2 < 1/4,$$

then there exists a constant $\gamma_0 > 0$, depending only on $\alpha\|Z\|^2$, such that

$$\|A^T u\| \geq \gamma_0\|u\| \qquad \forall u \in \mathbb{R}^N.$$

Proof. We decompose A^T into

$$A^T = I + \alpha Z^T L Z X P_{\mathcal{U}} = \big[I - P_{\mathcal{U}}\big] + P_{\mathcal{U}}\big[I - \alpha Z^T L Z X P_{\mathcal{U}}\big],$$

where we have used the fact that $P_{\mathcal{U}} L = L$ and that $P_{\mathcal{U}}$ commutes with Z. Since $P_{\mathcal{U}}$ is an orthogonal projection we obtain, again using $P_{\mathcal{U}} L = L$,

$$\|A^T v\|^2 = \|[1 - P_{\mathcal{U}}]v\|^2 + \|[I - \alpha Z^T L Z X] P_{\mathcal{U}} v\|^2. \tag{32}$$

We will show next that

$$\|[1 - \alpha Z^T L Z X]w\|^2 \geq (1-\epsilon)\|w\|^2 \qquad \forall w \in \mathcal{U}, \tag{33}$$

where $\epsilon \in (0,1)$ is defined in (37) and depends only on $\alpha\|Z\|^2$, but not on N or $\mathcal{A}$. Hence, (33) combined with (32), gives the desired result

$$\|A^T v\|^2 \geq \min(1, 1-\epsilon)(\|[1 - P_{\mathcal{U}}]v\|^2 + \|P_{\mathcal{U}} v\|^2) = \gamma_0\|v\|^2,$$

with $\gamma_0 = \sqrt{1-\epsilon}$.

Proof of (33). We begin by splitting the operator, using $X^2 = X$, into

$$\begin{aligned}
[I - \alpha Z^T L Z X] &= X[I - \alpha Z^T L Z X] + [I - X][I - \alpha Z^T L Z X] \\
&= X[I - \alpha Z^T L Z]X + [I - X][I - \alpha Z^T L Z X] \\
&=: S_1 + S_2.
\end{aligned}$$

Since X is an orthogonal projection, we have, for any $w \in \mathcal{U}$,

$$\big\|[I - \alpha Z^T L Z X]w\big\|^2 = \|S_1 w\|^2 + \|S_2 w\|^2. \tag{34}$$

Estimating S_1. Since $S_1 = X[I - \alpha Z^T L Z]X$ is a symmetric operator, the following variational bound is found using the fact that $0 \leq \langle Lx, x\rangle \leq 4$. We obtain

$$\begin{aligned}
\big\langle X[I - \alpha Z^T L Z]Xw, w\big\rangle &= \|Xw\|^2 - \alpha\big\langle LZXw, ZXw\big\rangle \\
&\geq \min\big(1, 1 - 4\alpha\|Z\|^2\big)\|Xw\|,
\end{aligned}$$

where the last equality follows by distinguishing the cases $\alpha < 0$ and $\alpha \geq 0$.

In summary, if $\alpha\|Z\|^2 < 1/4$, then we have the $N, \mathcal{A}$-independent bound

$$\|S_1 w\|^2 \geq \big[\min(1, 1 - 4\alpha\|Z\|^2)\big]^2\|Xw\|^2 \qquad \forall w \in \mathbb{R}^N. \tag{35}$$

Estimating S_2. Due to the good estimate on S_1 we only need fairly rough estimates on the term $\|S_2 w\|^2$. Application of the Cauchy–Schwartz inequality and a weighted Cauchy inequality provides the estimate

$$\|S_2 w\|^2 \geq (1-\epsilon)\|[I-X]w\|^2 + (1-\epsilon^{-1})\alpha^2\|[I-X][Z^T LZ]Xw\|^2,$$

for any $\epsilon \in (0,1)$. Using the fact that $I - X$ is an orthogonal projection, $\|L\| \leq 4$, we can further estimate

$$\|S_2 w\|^2 \geq (1-\epsilon)\|[I-X]w\|^2 + (1-\epsilon^{-1})16\|Z\|^4\alpha^2\|Xw\|^2. \tag{36}$$

Combining the estimates. If we define $\tilde{\alpha} = 4\alpha\|Z\|^2$, and insert (35) and (36) into (34), we obtain, for all $w \in \mathcal{U}$,

$$\begin{aligned}\|[I-\alpha Z^T LZX]w\|^2 &\geq \big\{\min(1,(1-\tilde{\alpha})^2) + (1-\epsilon^{-1})\tilde{\alpha}^2\big\}\|Xw\|^2 + (1-\epsilon)\|[I-X]w\|^2 \\ &\geq \min\big\{\min(1,(1-\tilde{\alpha})^2) + (1-\epsilon^{-1})\tilde{\alpha}^2, 1-\epsilon\big\}\|w\|^2,\end{aligned}$$

for any $\epsilon \in (0,1)$. Since $\min(1,(1-\tilde{\alpha})^2) > 0$ it is clear that choosing ϵ sufficiently close to 1 gives a positive lower bound. To optimize this constant with respect to ϵ, we have to choose ϵ to equalize the two competitors in the outer min formula. The resulting choice is

$$\epsilon = \begin{cases} \sqrt{\tilde{\alpha}^2 + \frac{1}{4}\tilde{\alpha}^4} - \frac{1}{2}\tilde{\alpha}^2, & \tilde{\alpha} \leq 0, \\ \tilde{\alpha} - \tilde{\alpha}^2 + \sqrt{2(\tilde{\alpha}^2 - \tilde{\alpha}^3) + \tilde{\alpha}^4}, & 0 < \tilde{\alpha} < 1, \end{cases} \tag{37}$$

which concludes the proof of (33). (As a matter of interest, $\epsilon \to 1$ as $\tilde{\alpha} \to 1$, $\epsilon = 0$ for $\tilde{\alpha} = 0$, and $\epsilon \to 1$ as $\tilde{\alpha} \to -\infty$.) □

4.3. **Estimates for the eigenvalues.** Using the similarity to a symmetric matrix that we have established in the previous section we can now give sharp bounds on the spectrum of L_0^{qcf}.

Theorem 12. *Suppose that* (25) *holds, then L_0^{qcf} has a real, ordered spectrum $(\lambda_j)_{j=1}^N$. If we denote the ordered eigenvalues of L^{a} and L^{c}, respectively, by $(\lambda_j^{\mathrm{a}})_{j=1}^N$ and $(\lambda_j^{\mathrm{c}})_{j=1}^N$ then*

$$\begin{aligned} &\lambda_j^{\mathrm{c}} \leq \lambda_j \leq \lambda_j^{\mathrm{a}}, && \textit{for } j = 1,\dots,N, \quad \textit{if } b(t) \geq 0, \quad \textit{and} \\ &\lambda_j^{\mathrm{a}} \leq \lambda_j \leq \lambda_j^{\mathrm{c}}, && \textit{for } j = 1,\dots,N, \quad \textit{if } b(t) \leq 0. \end{aligned}$$

Proof. We know from Theorem 10 that L_0^{qcf} is diagonalizable and that it is similar to the self-adjoint operator L^{sym} defined in (29), which has a real spectrum that is identical to the spectrum of L_0^{qcf}. We will next show that, for all $u \in \mathbb{R}^N$,

$$\begin{aligned} &\langle L^{\mathrm{c}}u, u, \rangle \leq \langle L^{\mathrm{sym}}u, u\rangle \leq \langle L^{\mathrm{a}}u, u\rangle, && \text{if } \sigma = 1, \quad \text{and} \\ &\langle L^{\mathrm{a}}u, u, \rangle \leq \langle L^{\mathrm{sym}}u, u\rangle \leq \langle L^{\mathrm{c}}u, u\rangle, && \text{if } \sigma = -1. \end{aligned} \tag{38}$$

From these inequalities, the min-max characterisation of eigenvalues [17, Sec. XIII.1] immediately gives the stated result.

To prove (38) we will take the following starting point:

$$\langle L^{\mathrm{sym}}u, u\rangle = \langle L^{\mathrm{c}}u, u\rangle + \sigma\langle Y^T XYu, u\rangle = \langle L^{\mathrm{c}}u, u\rangle + \sigma\langle XY^T u, XY^T u\rangle. \tag{39}$$

From here on, we treat the cases $\sigma = 1$ and $\sigma = -1$ separately.

Case 1: $\sigma = 1$. Using (39) and the fact that $Y^T Y = L^{\rm a} - L^{\rm c}$, we have

$$\langle L^{\rm sym} u, u\rangle \le \langle L^{\rm c} u, u\rangle + \langle Y^T u, Y^T u\rangle = \langle L^{\rm c} u, u\rangle + \langle [L^{\rm a} - L^{\rm c}]u, u\rangle = \langle L^{\rm a} u, u\rangle.$$

For the lower bound we use (39) and the fact that $\langle XY^T u, XY^T u\rangle$ is non-negative to obtain

$$\langle L^{\rm sym} u, u\rangle \ge \langle L^{\rm c} u, u\rangle.$$

Case 2: $\sigma = -1$. The idea for $\sigma = -1$ is essentially that the roles of $L^{\rm a}$ and $L^{\rm c}$ are reversed. Note that, now, $Y^T Y = L^{\rm c} - L^{\rm a}$. Hence, for the upper bound, we get

$$\langle L^{\rm sym} u, u\rangle \le \langle L^{\rm c} u, u\rangle,$$

whereas, for the lower bound, we get

$$\langle L^{\rm sym} u, u\rangle \ge \langle L^{\rm c} u, u\rangle - \langle Y^T u, Y^T u\rangle = \langle L^{\rm c} u, u\rangle - \langle [L^{\rm c} - L^{\rm a}]u, u\rangle = \langle L^{\rm a} u, u\rangle. \qquad \square$$

4.4. **The case of non-positive coefficients.** For many of the common interaction potentials, such as the Lennard–Jones potential, $\phi(r) = Ar^{-12} + Br^{-6}$, or the Morse potential, $\phi(r) = \exp(-2\alpha(r - r_0)) + 2\exp(-\alpha(r - r_0))$, there exists a minimal strain F_* such that, for all $F \ge F_*$, we have

$$\phi''_{rF} \le 0 \qquad \text{for} \quad r = 2, \dots, R. \tag{40}$$

In most cases, it is reasonable to assume that the macroscopic strain F remains in this region, as it would require extreme compressive forces to violate it. Hence, for the remainder of the section, we will assume that (40) is satisfied. The following two lemmas reduce this case to the one studied earlier in this section.

Lemma 13. *Suppose that* (40) *holds, then $b(t) \ge 0$ in $\mathcal{T}$.*

Proof. Similarly as in the proof of Lemma 7 we rewrite $b(t)$ in the form

$$\begin{aligned} b(t) &= \sum_{r=2}^{R} \phi''_{rF} \big[(t^r - 1)(t^{-r} - 1) - r^2 (t-1)(t^{-1} - 1)\big] \\ &= (t-1)(t^{-1}-1) \sum_{r=2}^{R} \phi''_{rF} \big[(t^{r-1} + t^{r-2} + \ldots + 1)(t^{-r+1} + t^{-r+2} + \ldots + 1) - r^2\big]. \end{aligned} \tag{41}$$

It is easy to see that $(t-1)(t^{-1}-1)$ is non-negative on $\mathcal{T}$, and moreover, for $t \in \mathcal{T}$,

$$(t^{r-1} + t^{r-2} + \ldots + 1)(t^{-r+1} + t^{-r+2} + \ldots + 1) = |t^{r-1} + t^{r-2} + \ldots + 1|^2 \le r^2. \tag{42}$$

Hence we obtain the stated result. $\square$

Lemma 14. *Suppose that* (40) *holds and that $\phi''_{RF} < 0$. Then* (25) *is satisfied with constants β_0 and β_1 that are independent of N and $\mathcal{A}$.*

Proof. The upper bound β_1 in (40) obviously exists since $b_1(t)$ is a continuous function on a compact set $\mathcal{T}$.

To show the existence of the lower bound it is sufficient to show that

$$b_1(t) > 0 \quad \text{for all } t \in \mathcal{T}. \tag{43}$$

Suppose that $b_1(t_1) \leq 0$ at some point $t_1 \in \mathcal{T}$. Then $b(t_1) \leq 0$ and hence at least one term in the definition of $b(t)$ (21) is non-positive. To be precise, there exists $r \in \{2, \ldots, R\}$ such that $\phi''_{rF} < 0$ and

$$(-\phi''_{rF})\left[r^2(t_1-1)(t_1^{-1}-1) - (t_1^r-1)(t_1^{-r}-1)\right] \leq 0$$

It follows from (41) and (42) that this may only happen at $t_1 = 1$. However, a striaght-forward computation shows that

$$b_1(1) = \lim_{t\to 1} \frac{r^2(t-1)(t^{-1}-1) - (t^r-1)(t^{-r}-1)}{\left[(t-1)(t^{-1}-1)\right]^2} = \frac{r^4-r^2}{12} > 0.$$

Hence no point $t_1 \in \mathcal{T}$ such that $b_1(t_1) \leq 0$ exists. □

We are now in a position to complete the proof of Theorem 5.

Proof of Theorem 5. Item (i) is a special case of Proposition 8, taking into account that, for non-positive coefficients, $b(t)$ defined in (21) is non-negative and Y_1 can therefore be chosen to be real. Item (ii) follows from Theorem 10 and Proposition 14. Item (iii) is established in Theorem 12. □

We conclude this section with a result that gives the sharp bounds on β_0, β_1 for the case of non-positive coefficients.

Proposition 15. *Let $b_1(t)$ be defined by* (24) *and suppose that* (40) *holds; then* (25) *holds with constants*

$$\beta_0^2 = \sum_{r=2}^{R}(-\phi''_{rF})\frac{2r^2+(-1)^r-1}{8}, \qquad \textit{and}$$
$$\beta_1^2 = \sum_{r=2}^{R}(-\phi''_{rF})\frac{r^2(r^2-1)}{12}.$$

The lower bound is attained at $t = -1$ and the upper bound is attained at $t = 1$.

The proof of this proposition is based on the following technical lemma.

Lemma 16. *For $r \in \mathbb{N}$, $r \geq 2$, let $f_r : (0, \frac{\pi}{2}] \to \mathbb{R}$ be defined as*

$$f_r(\beta) := \frac{1}{\sin^2\beta}\left(r^2 - \frac{\sin^2 r\beta}{\sin^2\beta}\right), \tag{44}$$

then

$$\inf_{0<|\beta|\le\frac{\pi}{2}} f_r(\beta) = f_r(\pi/2) = r^2 - \frac{1-(-1)^r}{2}, \qquad \text{and} \tag{45}$$

$$\sup_{0<|\beta|\le\frac{\pi}{2}} f_r(\beta) = \lim_{\beta\to 0} f_r(\beta) = \frac{1}{3}r^2(r^2-1). \tag{46}$$

Proof. Proof of (45). First, notice that

$$f_r(\pi/2) = r^2 - \sin^2\frac{r\pi}{2} = r^2 - \frac{1-(-1)^r}{2},$$

which proves that the left-hand side of (45) is not larger than the right-hand side. To prove the that $f_r(\beta) \ge f_r(\pi/2)$ for all β, transform

$$\begin{aligned} f_r(\beta) = &\ \frac{1}{\sin^2\beta}\left(r^2 - \frac{\sin^2 r\beta}{\sin^2\beta}\right) = \frac{1}{\sin^2\beta}\left(r^2 - r^2\sin^2\beta - \frac{\sin^2 r\beta}{\sin^2\beta}\right) + r^2 \\ = &\ \frac{1}{\sin^2\beta}\left(r^2\cos^2\beta - \frac{\sin^2 r\beta}{\sin^2\beta}\right) + r^2 = \frac{1}{\sin^2\beta}\left(\frac{r^2\sin^2 2\beta}{4\sin^2\beta} - \frac{\sin^2 r\beta}{\sin^2\beta}\right) + r^2 \\ &\ = \frac{r^2}{\sin^4\beta}\left(\frac{\sin^2 2\beta}{4} - \frac{\sin^2 r\beta}{r^2}\right) + r^2 \end{aligned} \tag{47}$$

and consider the three cases: $0 < \beta < \frac{\pi}{2r}$, $\frac{\pi}{2r} \le \beta \le \frac{\pi}{2} - \frac{\pi}{2r}$, and $\frac{\pi}{2} - \frac{\pi}{2r} < \beta \le 1$.

Case 1. ($0 < \beta \le \frac{\pi}{2r}$) Further transform the function $f_r(\beta)$ in (47):

$$f_r(\beta) = \frac{r^2\beta^2}{\sin^4\beta}\left(\operatorname{sinc}^2 2\beta - \operatorname{sinc}^2 r\beta\right) + r^2.$$

The expression in the brackets is positive since $\operatorname{sinc} x = \frac{\sin x}{x}$ is a decreasing function for $0 < x \le \pi/2$. This proves $f_r(\beta) \ge r^2 \ge f_r(\pi/2)$.

Case 2. ($\frac{\pi}{2r} \le \beta \le \frac{\pi}{r} - \frac{\pi}{2r}$) In this case $\sin 2\beta \ge \frac{2}{r}$, hence

$$\begin{aligned} f_r(\beta) &= \frac{1}{\sin^2\beta}\left(\frac{r^2\sin^2 2\beta}{4\sin^2\beta} - \frac{\sin^2 r\beta}{\sin^2\beta}\right) + r^2 \\ &\ge \frac{1}{\sin^2\beta}\left(\frac{1}{\sin^2\beta} - \frac{\sin^2 r\beta}{\sin^2\beta}\right) + r^2 \ge r^2 \ge f_r(\pi/2). \end{aligned}$$

Case 3. ($\frac{\pi}{2} - \frac{\pi}{2r} < \beta \le 1$) Denote $x = \frac{\pi}{2} - \beta$ ($0 \le x < \frac{\pi}{2r}$) and consider the two different subcases: r is even/odd.

Case 3.1. (r is even) In this case $\sin\beta = \cos x$, $\sin 2\beta = \sin 2x$, and $\sin^2 r\beta = \sin^2(rx)$. Hence $f_r(\theta)$ as expressed in (47) takes the form

$$\begin{aligned} f_r(\beta) &= \frac{r^2}{\cos^4 x}\left(\frac{\sin^2 2x}{4} - \frac{\sin^2 rx}{r^2}\right) + r^2 \\ &= \frac{r^2x^2}{\cos^4 x}\left(\operatorname{sinc}^2 2x - \operatorname{sinc}^2 rx\right) + r^2 \ge r^2 = f_r(\pi/2). \end{aligned}$$

Case 3.2. (r is odd) In this case $\sin\beta = \cos x$, $\sin^2 2\beta = \sin^2 2x$, and $\sin^2 r\beta = \cos^2(rx)$. Hence (47) transforms into

$$\begin{aligned} f_r(\beta) &= \frac{r^2}{\cos^4 x}\left(\frac{\sin^2 2x}{4} - \frac{\cos^2 rx}{r^2}\right) + r^2 \ge r^2 - \left(\frac{\cos^2 x}{\cos rx}\right)^{-2} = r^2 - \left(\frac{1+\cos 2x}{2\cos rx}\right)^{-2} \\ &\ge r^2 - \left(\frac{1}{2}+\frac{1}{2}\right)^{-2} = r^2 - 1 = f_r(\pi/2). \end{aligned}$$

Here we used the fact that $1 \ge \cos 2x \ge \cos rx$ $(0 \le x < \frac{\pi}{2r})$.

Proof of (46). First compute

$$\begin{aligned} \lim_{\beta\to 0} f_r(\beta) &= \lim_{\beta\to 0}\frac{r^2\sin^2\beta - \sin^2 r\beta}{\sin^4\beta} = \lim_{\beta\to 0}\frac{r^2\left(\beta^2 - \beta^4/3\right) - \left(r^2\beta^2 - r^4\beta^4/3\right) + O(\beta^6)}{\beta^4} \\ &= -\frac{r^2}{3} + \frac{r^4}{3} = \frac{1}{3}r^2(r^2-1). \end{aligned}$$

To prove the inequality $f_r(\beta) \le \frac{1}{3}r^2(r^2-1)$ consider the two cases: $\frac{\pi}{r} \le \beta \le \frac{\pi}{2}$ and $0 < \beta < \frac{\pi}{r}$.

Case 1. $(\frac{\pi}{r} \le \beta \le \frac{\pi}{2})$ In this case (46) follows directly from the following computation:

$$\begin{aligned} \frac{1}{3}r^2(r^2-1)\big[f_r(\beta)\big]^{-1} &\ge \frac{1}{3}r^2(r^2-1)\left[\frac{r^2}{\sin^2\beta}\right]^{-1} = \frac{1}{3}(r^2-1)\,\sin^2\beta \\ &\ge \frac{1}{3}(r^2-1)\,\sin^2\frac{\pi}{r} \ge \frac{1}{3}(r^2-1)\left(\frac{2}{r}\right)^2 = \frac{4r^2-4}{3r^2} \ge \frac{4}{3} - \frac{1}{3} = 1. \end{aligned}$$

Case 2. $(0 < \beta < \frac{\pi}{r})$ We need to prove

$$r^{-2}\left(f_r(\beta) - \frac{1}{3}r^2(r^2-1)\right) \;=\; \frac{f_r(\beta)}{r^2} - \frac{1}{3}(r^2-1) \;\le\; 0 \qquad (\forall\beta\in(0,\pi/r)) \tag{48}$$

for integer r, but instead we prove that it is valid for all real values of $r \in [2,\infty)$.

First, notice that the following calculation

$$\left.\frac{f_r(\beta)}{r^2} - \frac{1}{3}(r^2-1)\right|_{r=2} = \frac{1}{4}\,\frac{1}{\sin^2\beta}\left(4 - \frac{\sin^2 2\beta}{\sin^2\beta}\right) - 1 = \frac{1}{4\sin^2\beta}\left(4 - 4\cos^2\beta\right) - 1 = 0$$

proves (48) for $r = 2$. As is shown below,

$$\frac{\partial}{\partial r}\left(\frac{f_r(\beta)}{r^2} - \frac{1}{3}(r^2-1)\right) \le 0 \qquad (\forall\beta\in(0,\pi/r)), \tag{49}$$

which concludes the proof of (48).

Proof of (49). We use the standard inequalities

$$\begin{aligned} \operatorname{sinc}'(x) &\ge -x/3, && \forall x \ge 0 \\ \cos x &\le \operatorname{sinc}^3(x) && \forall x \in [0,\pi] \end{aligned}$$

and obtain

$$\frac{\partial}{\partial r}\left(\frac{f_r(\beta)}{r^2}\right) = \frac{\partial}{\partial r}\left(\frac{1}{\sin^2\beta} - \frac{\sin^2 r\beta}{r^2\sin^4\beta}\right) = -\frac{\partial}{\partial r}\left(\frac{\beta^2\,\mathrm{sinc}^2\, r\beta}{\sin^4\beta}\right)$$
$$= -\frac{2\beta^3\,\mathrm{sinc}\, r\beta\,\mathrm{sinc}'\, r\beta}{\sin^4\beta} \le \frac{2\beta^3\,\mathrm{sinc}\, r\beta\,(r\beta)}{3\sin^4\beta},$$

and hence

$$\frac{\partial}{\partial r}\left(\frac{f_r(\beta)}{r^2} - \frac{1}{3}(r^2-1)\right) \le \frac{2\beta^3\,\mathrm{sinc}\, r\beta\,(r\beta)}{3\sin^4\beta} - \frac{2r}{3} = \frac{2r}{3}\left(\frac{\beta^4\,\mathrm{sinc}\, r\beta}{\sin^4\beta} - 1\right)$$
$$\le \frac{2r}{3}\left(\frac{\beta^4\,\mathrm{sinc}\, 2\beta}{\sin^4\beta} - 1\right) = \frac{2r}{3}\left(\frac{\beta^3\cos\beta}{\sin^3\beta} - 1\right) \le 0. \qquad \square$$

Proof of Proposition 15. To reduce the problem to the statement of Lemma 16 we make the substitution $\beta = e^{2i\beta}$, $-\pi/2 < \theta < \pi/2$, which gives

$$\begin{aligned} b(t) &= \sum_{r=2}^{R} (-\phi''_{rF})\,\frac{r^2(t-1)(t^{-1}-1) - (t^r-1)(t^{-r}-1)}{\big[(t-1)(t^{-1}-1)\big]^2} \\ &= \sum_{r=2}^{R} (-\phi''_{rF})\,\frac{r^2(e^{2i\beta}-1)(e^{-2i\beta}-1) - (e^{2ir\beta}-1)(e^{-2ir\beta}-1)}{\big[(e^{2i\beta}-1)(e^{-2i\beta}-1)\big]^2} \\ &= \sum_{r=2}^{R} (-\phi''_{rF})\,\frac{r^2\,4\sin^2\beta - 4\sin^2 r\beta}{16\sin^4\beta} = \sum_{r=2}^{R} (-\phi''_{rF})\,\frac{f_r(\beta)}{4}. \end{aligned}$$

Application of Lemma 16 gives Proposition 15. $\square$

5. Analysis of Preconditioned L_0^{qcf} Operators

In this final section we present two further interesting applications of our foregoing analysis. First, we discuss the GMRES solution of a linearized QCF system. We rigorously establish some conjectures used in [6] and briefly discuss their consequences. Second, we prove a new stability result for the linearized QCF operator in a discrete Sobolev norm, which we hope will become a useful tool for future analyses of the QCF method.

We assume throughout this section that (28) holds and that Y_1 is defined by (26). Moreover, we recall the definition of L^{sym} from (29). Since the results are fairly straightforward corollaries from our analysis in Section 4 we will derive them in a less formal manner.

5.1. **GMRES-Solution of the QCF system.** We consider the linearized QCF system

$$L_0^{\mathrm{qcf}} u = f, \tag{50}$$

where $f \in \mathcal{U}$, which is to be solved for $u \in \mathcal{U}$. If this system is solved using the GMRES algorithm (see [19] for a general introduction and [6] for a detailed discussion of using GMRES for solving the QCF system), then standard estimates on GMRES convergence [19],

along with the analysis of the previous sections, show that the residual of the m-th iterate, $r^{(m)} = f - L_0^{\rm qcf} u^{(m)}$, satisfies the bound

$$\|r^{(m)}\| \le 2\,\mathrm{cond}(V^{\rm qcf}) \left(\frac{1-\sqrt{\gamma}}{1+\sqrt{\gamma}} \right)^m \|r^{(0)}\|,$$

where $\gamma = \lambda_2/\lambda_N = O(1/N^2)$ (see also [6, Prop. 22]). The fraction λ_2/λ_N is used instead of λ_1/λ_N since we are solving the system in $\mathcal{U}$. This convergence is rather slow and hence two variants of preconditioned GMRES (P-GMRES) algorithms were suggested in [6]. The preconditioner used was the negative Laplacian L. We will use the preconditioner L_1 instead of L, however, this is purely for the sake of a consistent notation since $L_1^{-1} L_0^{\rm qcf} = L^{-1} L_0^{\rm qcf}$ (note that $\mathrm{rg}\, L_0^{\rm qcf} = \mathcal{U}$ and that L^{-1} is well-defined on $\mathcal{U}$).

The first variant of P-GMRES that was considered in [6] was the standard left-preconditioned GMRES algorithm where GMRES is applied to the preconditioned system

$$L_1^{-1} L_0^{\rm qcf} u = L_1^{-1} f. \tag{51}$$

To obtain convergence rates, we require bounds on the eigenvalues and eigenbasis of $L_1^{-1} L_0^{\rm qcf}$ (see [6, Sec. 6.2]).

The second variant considers again the left-preconditioned system (51) but this time the residual is minimized in the norm induced by the operator L_1. The convergence rates of the resulting method are governed by the spectrum and eigenbasis of the operator $L_1^{-1/2} L_0^{\rm qcf} L_1^{-1/2}$ (see [6, Sec. 6.3]).

5.1.1. *Diagonalization.* We consider $L_1^{-1/2} L_0^{\rm qcf} L_1^{-1/2}$ first. Using (29), and the fact that $L_1^{-1/2}$ commutes with $L_1 Y_1$, we obtain

$$[L_1 Y_1][L_1^{-1/2} L_0^{\rm qcf} L_1^{-1/2}][L_1 Y_1]^{-1} = L_1^{-1/2} L^{\rm sym} L_1^{-1/2} = \tilde{V}^{\rm sym} \tilde{\Lambda} (\tilde{V}^{\rm sym})^T,$$

where $\tilde{\Lambda}$ is the real diagonal matrix of eigenvalues and $\tilde{V}^{\rm sym}$ an orthonormal matrix of eigenvectors of $L_1^{-1/2} L^{\rm sym} L_1^{-1/2}$. Hence, we conclude that $L_1^{-1/2} L_0^{\rm qcf} L_1^{-1/2}$ is diagonalizable with real spectrum $\tilde{\Lambda}$:

$$[L_1^{-1/2} L_0^{\rm qcf} L_1^{-1/2}][Y_1^{-1} L_1^{-1} \tilde{V}^{\rm sym}] = [Y_1^{-1} L_1^{-1} \tilde{V}^{\rm sym}] \tilde{\Lambda}. \tag{52}$$

Multiplying the equation by $L_1^{-1/2}$, we obtain

$$[L_1^{-1} L_0^{\rm qcf}][Y_1 L_1^{-3/2} \tilde{V}^{\rm sym}] = [Y_1^{-1} L_1^{-3/2} \tilde{V}^{\rm sym}] \tilde{\Lambda}, \tag{53}$$

thus showing that also $L_1^{-1} L_0^{\rm qcf}$ is diagonalizable with the same real spectrum $\tilde{\Lambda}$. We note that this rigorously establishes a variant of [6, Conjecture 10].

5.1.2. *Condition number bounds.* Using the fact that $\tilde{V}^{\rm sym}$ is orthogonal, and Lemma 9 to bound $\mathrm{cond}(Y_1) \le \beta_1/\beta_0$, we can obtain the following upper bounds on the condition number of the matrices of eigenvectors:

$$\mathrm{cond}(Y_1^{-1} L_1^{-1} \tilde{V}^{\rm sym}) \lesssim N^2 \beta_1/\beta_0, \quad \text{and} \tag{54}$$

$$\mathrm{cond}(Y_1^{-1} L_1^{-3/2} \tilde{V}^{\rm sym}) \lesssim N^{3/2} \beta_1/\beta_0. \tag{55}$$

This rigorously establishes [6, Conjectures 12 and 13].

Since these bounds are not uniform in N the question arises whether we can define a better scaling for the eigenvectors to improve them. Note, however, that [7, Thm. 4.3] implies that $\mathrm{cond}(L_0^{\rm qcf}) \gtrsim N^{1/2}$, and hence no choice of eigenbasis can achieve an upper bound in (54) that is uniform in N. Moreover, numerical experiments in [6, Sec. 3, Figs. 2 and 3] indicate that our bounds may be optimal.

5.1.3. *Eigenvalue bounds.* To establish convergence rates for the P-GMRES solution of the QCF system, we still need to obtain bounds on the eigenvalues contained in $\tilde\Lambda$. Let $(\tilde\lambda_n)_{n=1}^N$ denote the ordered eigenvalues of $\tilde\Lambda$, and let $(\tilde\lambda_n^{\rm a})_{n=1}^N$ and $(\tilde\lambda_n^{\rm c})_{n=1}^N$ denote, respectively, the ordered eigenvalues of $L^{\rm a}$ and $L^{\rm c}$. Since $L^{\rm c} = W_F'' L$, we know that

$$\tilde\lambda_1^{\rm c} = 0, \quad \text{and} \quad \tilde\lambda_n^{\rm c} = W_F'' \quad \text{for } n = 2, \dots, N.$$

In view of Remark 4, replacing u by $L_1^{-1/2}u$ in the formulas, we obtain that

$$\begin{aligned} &\text{either} \qquad \big\langle [L_1^{-1/2} L^{\rm a} L_1^{-1/2}]u, u \big\rangle \geq \big\langle [L_1^{-1/2} L^{\rm c} L_1^{-1/2}]u, u \big\rangle \qquad \forall u \in \mathcal{U}, \\ &\text{or} \qquad \big\langle [L_1^{-1/2} L^{\rm a} L_1^{-1/2}]u, u \big\rangle \leq \big\langle [L_1^{-1/2} L^{\rm c} L_1^{-1/2}]u, u \big\rangle \qquad \forall u \in \mathcal{U}. \end{aligned}$$

Hence, we can repeat the proof of Theorem 12 verbatim to show that

$$\min(\tilde\lambda_n^{\rm a}, \tilde\lambda_n^{\rm c}) \leq \tilde\lambda_n \leq \max(\tilde\lambda_n^{\rm a}, \tilde\lambda_n^{\rm c}) \qquad \text{for } n = 1, \dots, N.$$

At this point we need to make an assumption on the stability of the atomistic system. We assume that the macroscopic strain F is chosen so that

$$c_0 \|u'\|^2 \leq \langle L^{\rm a} u, u \rangle \leq c_1 \|u'\|^2 \qquad \forall u \in \mathcal{U}. \tag{56}$$

The upper bound can be obtained in a straightforward computation that gives a constant c_1 depending only on the coefficients ϕ_{rF}'', $r = 1, \dots, R$. The lower bound means that the homogeneous deformation Fx lies in the region of stability of the atomistic energy (see [5] for a detailed discussion of this point, in particular, that c_0 is indeed independent of N). For example, in the case of non-positive coefficients Remark 4 shows that this bound holds with $c_0 = W_F''$, and that in the case $R = 2$ one can choose $c_0 = \min(W_F'', \phi_F'')$.

Upon noting that the stability assumption (56) is equivalent to the statement that $\tilde\lambda_2^{\rm a} \geq c_0$ and $\tilde\lambda_N^{\rm a} \leq c_1$, we can now deduce that

$$\min(c_0, W_F'') \leq \tilde\lambda_n \leq \max(c_1, W_F''),$$

which are bounds that are independent of N and $\mathcal{A}$.

5.1.4. *Convergence rates for P-GMRES.* From the foregoing discussion we obtain the following convergence rates for the P-GMRES solution of (50) (see [6, Sec. 6.2 and Sec. 6.3] for details of these derivations):

For the standard left-preconditioned GMRES algorithm we obtain bounds on the preconditioned residual,

$$\|L_1^{-1} r^{(m)}\| \leq C N^3 q^m \|L_1^{-1} r^{(0)}\|, \tag{57}$$

where $C > 0$ and $q \in (0, 1)$ are independent of N and $\mathcal{A}$.

For the left-preconditioned P-GMRES algorithm, which minimizes the preconditioned residual in the norm induced by L_1, we obtain

$$\|L_1^{-1/2} r^{(m)}\| \leq C N^2 q^m \|L_1^{-1/2} r^{(0)}\|, \tag{58}$$

where $C \geq 0$ and $q \in (0,1)$ are independent of N and $\mathcal{A}$.

We also note that a finer analysis (see [6, Sec. 6.2 and 6.3]) shows that both variants of P-GMRES reduce the residual to zero in at most $O(\#\mathcal{A})$ iterations.

5.2. **Stability of $L_0^{\rm qcf}$ in $\mathcal{U}^{2,2}$.** We define the discrete Sobolev-type norm

$$\|u\|_2 = \|Lu\| \qquad \text{for } u \in \mathbb{R}^N,$$

which is a norm on the space $\mathcal{U}$ of mean-zero functions and denote the space $\mathcal{U}$ equipped with $\|\cdot\|_2$ by $\mathcal{U}^{2,2}$. Moreover, we denote the space $\mathcal{U}$ equipped with the norm $\|\cdot\| =: \|\cdot\|_0$ by $\mathcal{U}^{0,2}$. We are interested in the question whether $L_0^{\rm qcf} : \mathcal{U}^{2,2} \to \mathcal{U}^{0,2}$ is stable, uniformly in N and $\mathcal{A}$.

To begin with, we note that

$$\|(L_0^{\rm qcf})^{-1}\|_{L(\mathcal{U}^{0,2},\mathcal{U}^{2,2})}^{-1} = \inf_{u \in \mathcal{U}\setminus\{0\}} \frac{\|L_0^{\rm qcf} u\|_0}{\|Lu\|_0} = \inf_{f \in \mathcal{U}\setminus\{0\}} \frac{\|L_0^{\rm qcf} L_1^{-1} f\|_0}{\|f\|_0};$$

thus, the question reduces to the analysis of the operator $L_0^{\rm qcf} L_1^{-1}$. Using the representation

$$L_0^{\rm qcf} = L^{\rm c} + \sigma P_{\mathcal{U}} X (L^{\rm a} - L^{\rm c}) = W_F'' L + \sigma P_{\mathcal{U}} X Y_1^T Y_1 L^2,$$

where Y_1 is defined in (26), we obtain

$$L_0^{\rm qcf} L_1^{-1} = W_F'' P_{\mathcal{U}} + \sigma P_{\mathcal{U}} X Y_1^T Y_1 L.$$

We now argue similar as in the proof of Theorem 9. On the space $\mathcal{U}$ the operator $W_F'' P_{\mathcal{U}} + P_{\mathcal{U}} X Y_1^T Y_1 L$ can be replaced by

$$W_F'' I + \sigma P_{\mathcal{U}} X Y_1^T Y_1 L.$$

For this modified operator Lemma 11 shows that it is invertible and provides uniform bounds on the inverse. Restricting the argument back to $\mathcal{U}$ we obtain the following theorem.

Theorem 17. *Suppose that $W_F'' > 0$, that (25) holds, and that $\sigma \beta_1^2 / W_F'' > -1/4$; then $L_0^{\rm qcf}$ is invertible and $\|(L_0^{\rm qcf})^{-1}\|_{L(\mathcal{U}^{0,2},\mathcal{U}^{2,2})}$ is bounded above by a constant that depends only on W_F'', β_0, β_1 (that is, on the coefficients $\phi_{rF}'', r = 1, \dots, R$) but is independent of N and of the choice of $\mathcal{A}$.*

6. Conclusion

We have established a comprehensive ℓ^2-theory of a linearized force-based quasicontinuum (QCF) operator making several conjectures from previous work [6, 7] regarding its spectrum and eigenbasis rigorous (at least up to a modification of the boundary conditions). We have given elementary derivations in the case of next-nearest neighbour interactions but have also provided proofs for arbitrary finite range interactions. Finally, as an immediate corollary of our analysis we have also obtained a new stability estimate in the space $\mathcal{U}^{2,2}$.

Our results heavily use the fact that the nonlinear QCF operator is linearized at a homogeneous deformation and a question of immediate relevance is whether our results can be generalized, at least partially, to linearizations around non-uniform states. Even

in small neighbourhoods of homogeneous deformations it is unclear whether this can be done.

Secondly, a generalization to 2D or 3D would have immense consequences as no approach to the analysis of QCF in 2D or 3D exists at this point.

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